#3

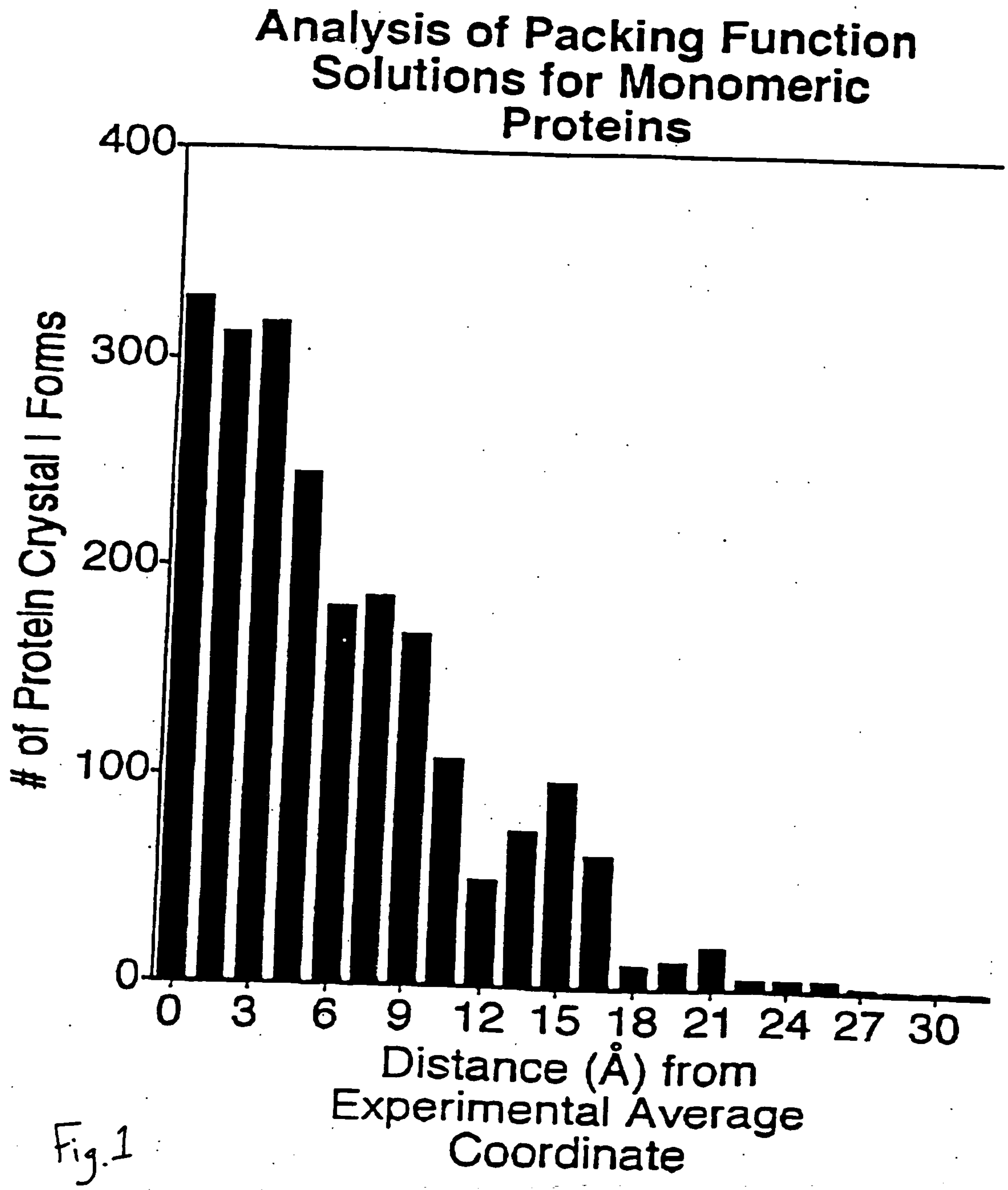

Analysis of Packing Function
Solutions for Monomeric
Proteins
# of Protein Crystal l Foms
400
300
200
100
0
0 3 6 9 12 15 18 21 24 27 30
Distance (Å) from
Experimental Average
Coordinate

Fig.1

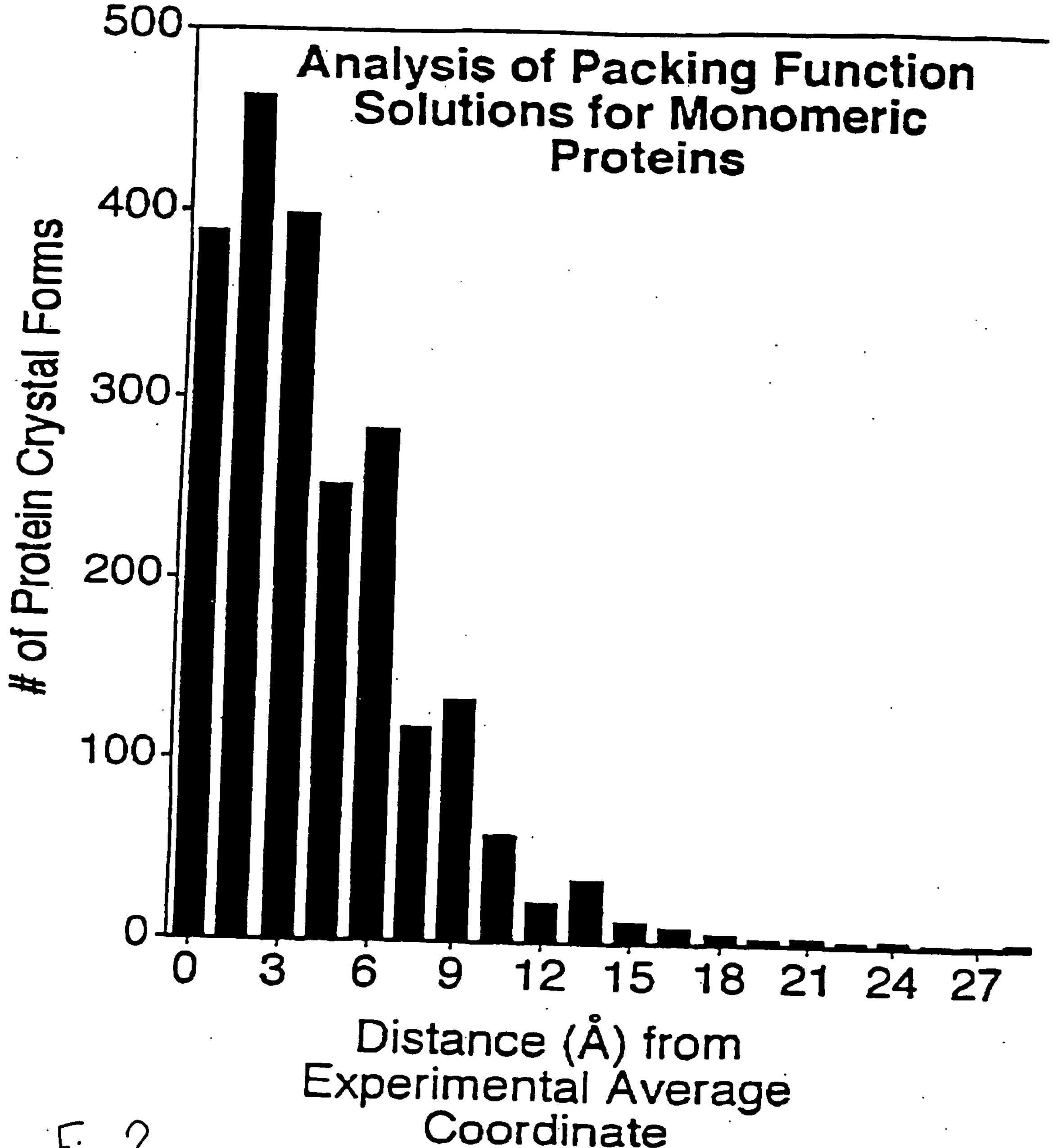

Analysis of Packing Function Solutions for Monomeric Proteins
500
400
300
200
100
0
# of Protein Crystal Forms
0
3
6
9
12
15
18
21
24
27
Distance (Å) from Experimental Average Coordinate

Fig. 2

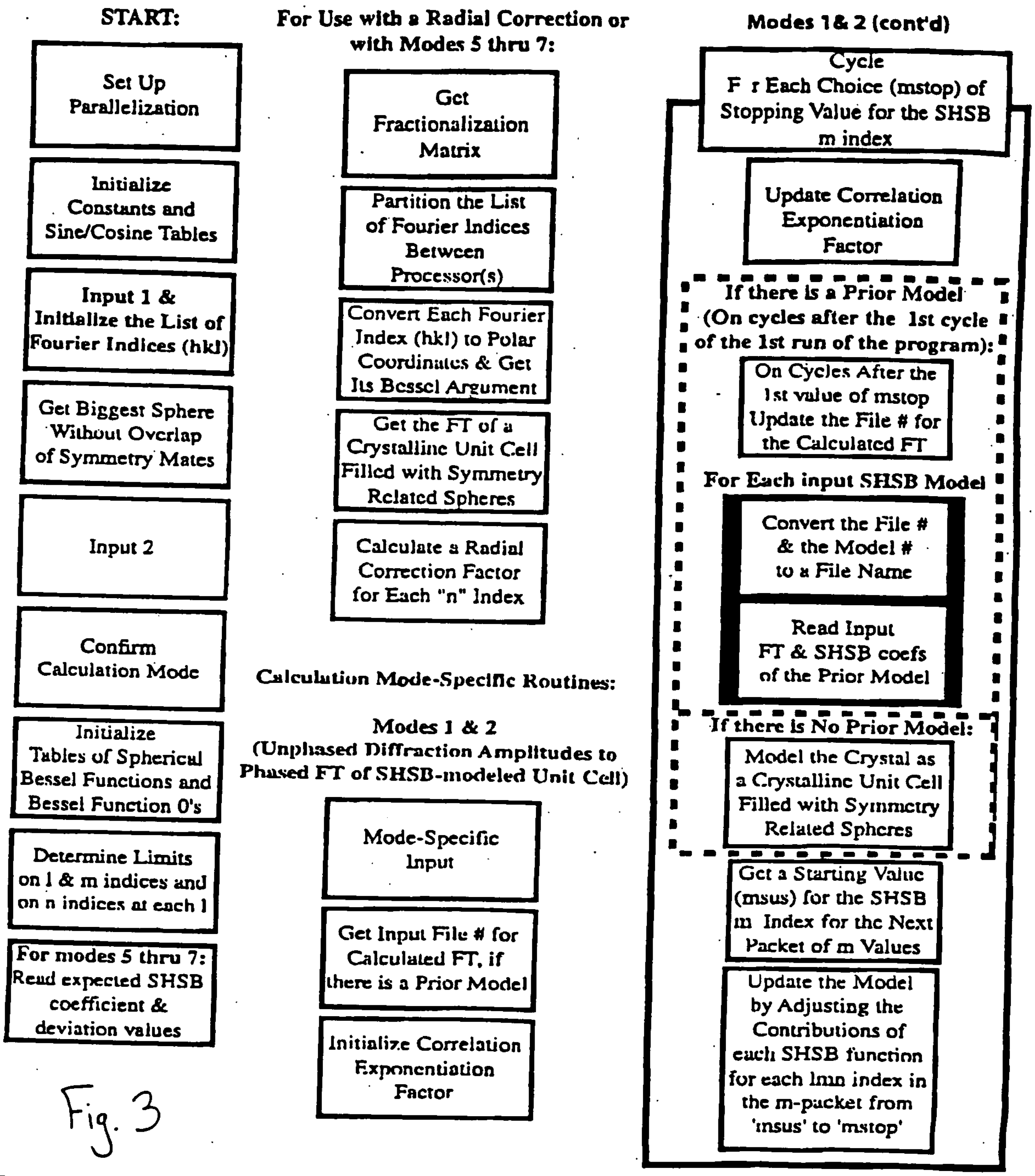


Fig. 3

Flow Chart for the Main Driver Program for "faizer": Options to compute a the FT of a SHSB Model of Crystal

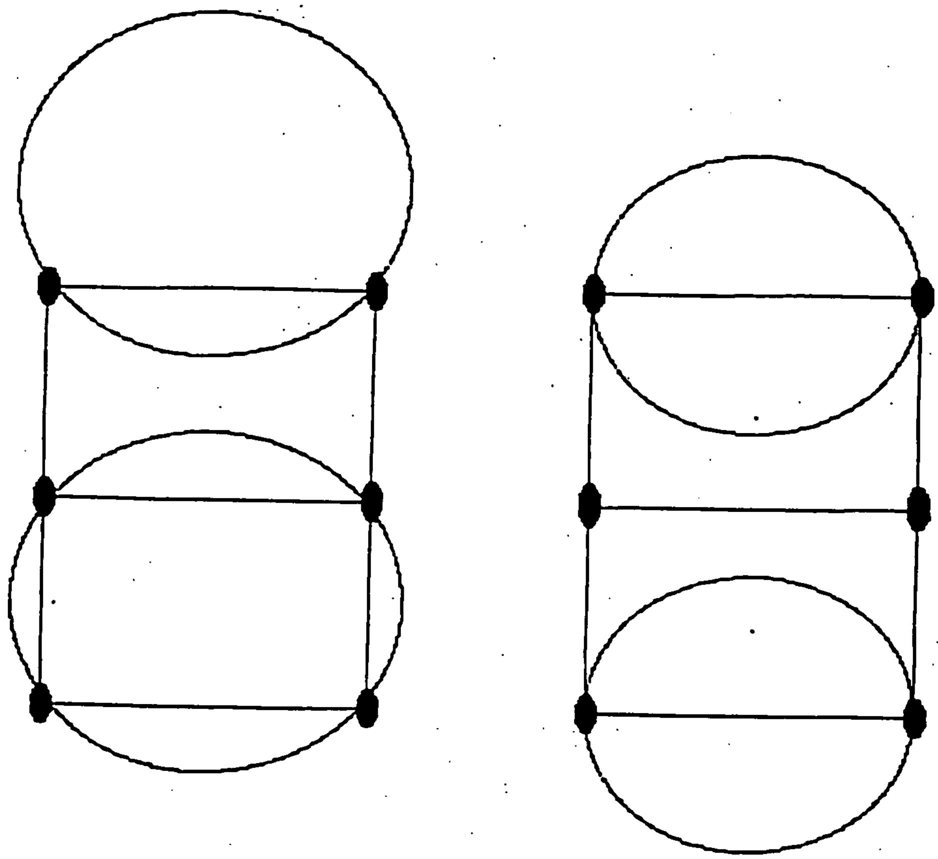


Figure 4 A schematic example: Two choices for filling the same portion of a crystal unit cell from an orthorhombic Spacegroup. Although the spheres on the right are smaller than those on the left, for some crystals, the local maximum in the packing on the right wold be the packing of maximal consistency with the crystallographic data.

Figure 4.

Initialize Fractionalization Matrix

Initialize the Equal Partitioning of the Fourier (hkl) Index between Processors

On 1st Cycle of 1st Run:
Prescale Observed Diffraction to that of a Unit Cell of Spheres

Define the First SHSB Index Triplet (lmn) for which to Consider Model |F|'s

Initialize for Index-by-Index Update of Origin-Centered SHSB Basis Function

Modes 4 & 5 only:
Initialize Buffers for Cumulative Update of Fourier Representation

Initialize Pointers to Stored Fourier Representations of Model and of Basis

Mode 3 only:
Get File Name from File # & Open It to Let SHSB Coefs. be Read

For each "m" Index (0 to maximum "m")

For Each hkl in this Partition:
Update "m" Recursion Formula for Fourier Representation of the Origin-Centered SHSB

For each "l" Index (present "m" to maximum "l")

For Each hkl in this Partition:
Update "l,m" Recursion Formula for Fourier Representation of the Origin-Centered SHSB

For each "n" Index (1 to maximum "n" for each "l")

For Each hkl in this Partition:
Update "n" Recursion Formula for Fourier Representation of the Origin-Centered SHSB

Depending on Mode:
Choose the # of Passes and # of Presumed Phase Angles Needed for the SHSB coef. with this SHSB index (lmn)

Set the Presumed Amplitude of the Origin-Centered SHSB Basis Function

FIRST PASS:

Initialize Registers: Overall Comparison of Correlation Coef. & Other Statistics

Renitialize Pointers to Storage Sites for Fourier Representations of the Full-Unit-Cell SHSB Basis

Parallel Processor Version:

Set # of calculations to: (# of presumed values of SHSB coef.'s phase) X (# of stored accumulated SHSB models for trial combination with this new SHSB component)

Given: # of processors, # of hkl partitions, # of calculations
Get: # of required rounds of trial combinations

For each round of trial combination on this processor

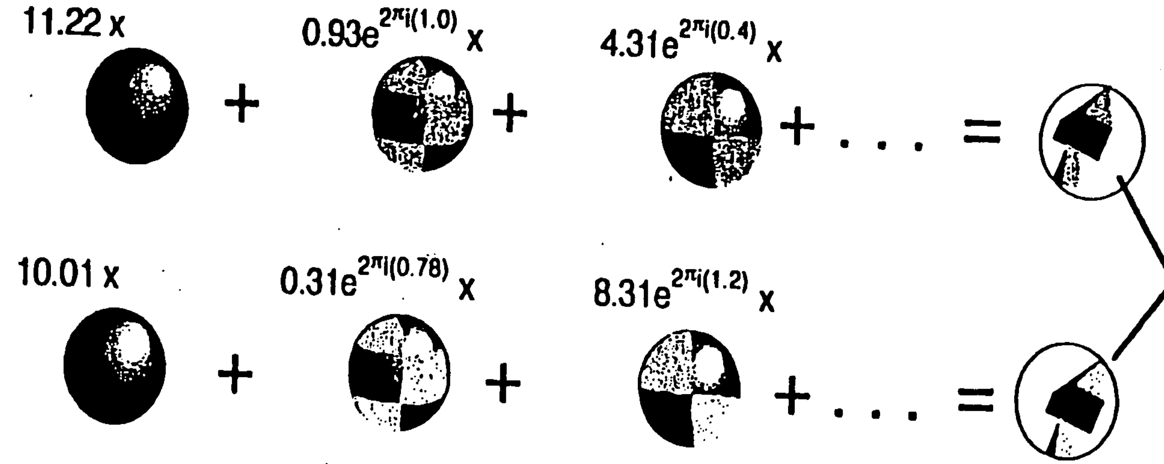
Single Processor Version: (Outer Loop)

For each presumed value of the SHSB coef.'s phase

Initialize Registers: Angular Comparison of Correlation Coef. & Other Statistics

Fig. 5

Identical Image from Expansions about Different Origins:



Symmetry Expanded Direct Space Basis Functions:

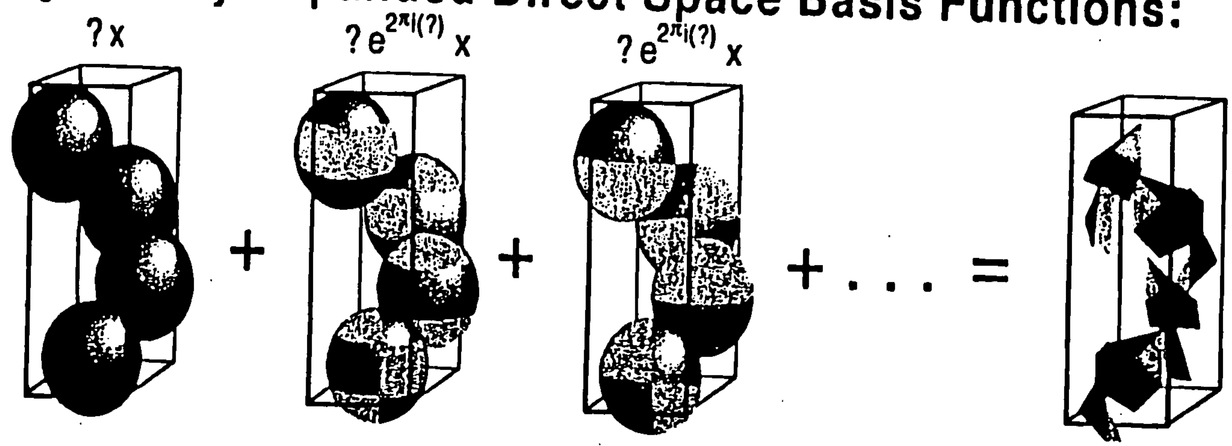
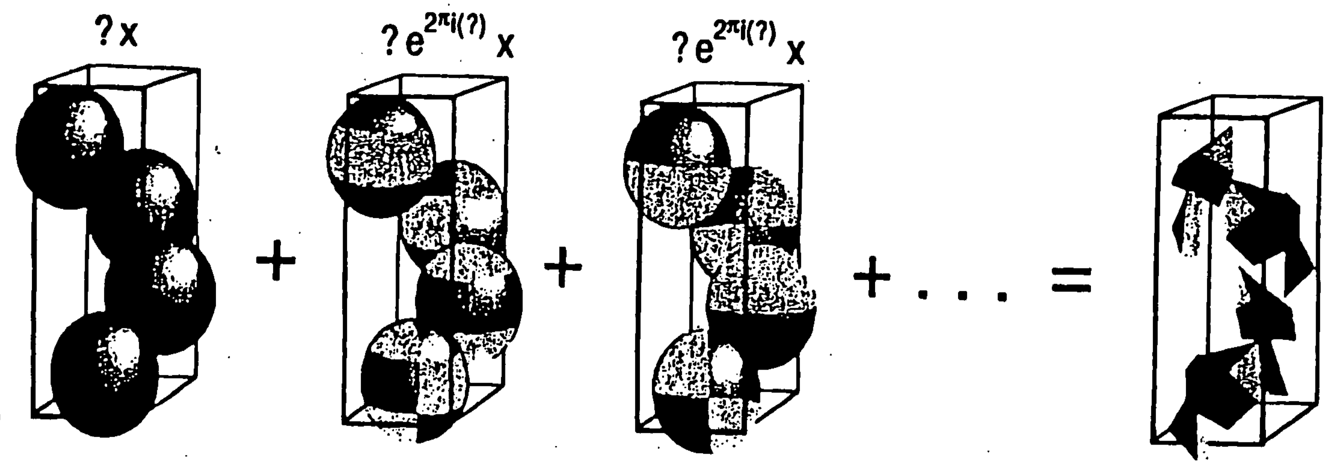


Fig. 6

With a properly chosen origin, 45-55% of the unit cell can be expanded. (Most protein crystals are > 45% solvent.)

Component Direct Space Basis Functions:



Component Fourier Transforms:

$$a_{001}F_{solo}^{001}(hkl) + a_{211}F_{solo}^{211}(hkl) + a_{111}F_{solo}^{111}(hkl) + \ldots = F_{obs}(hkl)$$

$$a_{001} = \Sigma_{hkl} F^{*}{}_{solo}^{001}(hkl)\, F_{obs}(hkl) \quad \text{[presume } \phi = 0.00 \text{ to start]}$$

$$F_{accum}(hkl) = a_{001}F_{solo}^{001}(hkl)$$

$$a_{211} = \Sigma_{hkl} F^{*}{}_{solo}^{211}(hkl)\, (|F_{obs}(hkl)| - |F_{accum}^{n}(hkl)|)e^{2\pi i \phi_{accum}^{n}(hkl)}$$

$$F_{accum}^{n+1}(hkl) = F_{accum}^{n}(hkl) + a_{211}F_{solo}^{211}(hkl)$$

Fig. 7